Title: Simulation of nanocomposites with a focus on effective electrical properties

Abstract: The continual development of stronger, lighter, and more efficient systems in civil, industrial, and military applications has fostered a long-standing drive for developing sophisticated composite materials in material science and engineering. To achieve the desired multi-functionalities, fiber-reinforced polymer-matrix composites are usually adopted for their superior electrical, mechanical, and thermal properties. These materials are ideal candidates for several applications, including aerospace, automotive, medical devices, coatings, and food packaging, just to name a few. Modeling and prediction of the nanocomposite properties are generally achieved using different statistical and micromechanical models. Introducing the polydispersity, filler alignment, and filler agglomeration into a finite element method is considered essential in accurately predicting the properties of the nanomaterials, thus eliminating the need for synthesizing each and every composite first to ascertain its properties. However, such polymer-based composite materials usually exhibit strong inhomogeneity, which makes it a grand challenge to simulate and optimize a specific property of the systems that rely on these materials. The primary objective of the proposed research work is to develop accurate and efficient solvers for analyzing nanocomposite materials. With this collaborative project serving as a cornerstone for investigating effective material properties, the successful completion of the proposed research will constitute a solid basis for designing and optimizing nanocomposite materials for aerospace and military applications. Computational modeling of the electromechanical response of nanocomposites incorporating different nanofillers is proposed to provide a better understanding of the effect of filler properties, the effect of filler alignment, the combination of fillers, nanofillers dispersion, filler agglomeration, and interactions with the host matrix. Such a study is needed to assess the effect of a wide variety of parameters that impact the thermal, mechanical and electrical properties of polymer nanocomposites. The proposed research study aims to achieve this goal by bringing together the disciplines of nanomechanics, electromagnetics, experimental and computational nanomaterials science.